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Du, T.; Smedskjær, Morten Mattrup; Li, H.; Bauchy, Mathieu

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(GOMD-S4-024-2018) Formation and Structure of Passivation Gels by Reactive Molecular Dynamics Simulations

T. Du^{*1}; M. M. Smedskjaer²; H. Li¹; M. Bauchy³

1. Harbin Institute of Technology, School of Civil Engineering, China 2. Aalborg University, Department of Chemistry and Bioscience, Denmark 3. University of California, Los Angeles, Department of Civil and Environmental Engineering, USA

The long-term dissolution rate (stage II) of nuclear waste immobilization glasses is thought to be controlled by the hydrated passivation gel that gradually forms on their surface. However, the mechanism of formation of such gel remains debated—i.e., precipitation from the solution or internal reorganization of the glass. Further, the mechanism of stage II dissolution (and its rate-limiting step) remains unclear. Here, based on reactive molecular dynamics simulations, we investigate the kinetics of formation and structure of several gels exhibiting varying compositions (i.e., varying Al/Si ratios) and formation mechanisms (i.e., solution precipitation or in situ glass reorganization). The influence of the composition and structure of the gel on the mobility of hydrated species is studied.